Wave Function and Pair Distribution Function of a Dilute Bose Gas

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The wave function of a dilute hard sphere Bose gas at low temperatures is discussed, emphasizing the formation of pairs. The pair distribution function is calculated for two values of $\sqrt{\rho a^3}$.

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The simplest nontrivial quantum mechanical many body problem that is precisely definable and at the same time subject to mathematical treatment is the dilute hard sphere Bose gas. In 1947 Bogoliubov studied this problem [1] and obtained its excitation spectrum. His method is now called [2] the Bogoliubov transformation. In 1957 Lee, Huang and Yang made [3] a detailed study of the problem and obtained its ground state energy in an asymptotic expansion:

$$\frac{E_0}{N} = (\frac{\hbar^2}{2m})4\pi a\rho[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + \ldots] \tag{1}$$

where N is the total number of particles, $\rho = N/\Omega$ is the density of particles, and a is the diameter of the sphere = scattering length.

With incredibly advanced modern technologies this system is now subject to experimental study. Many beautiful results [4] have been obtained, about equation (1) and about the excitation spectrum. We want to point out in this brief note that perhaps further interesting experimental exploration could be made to further clarify properties of the ground state. Throughout this note we follow the notation of reference [3].

WAVE FUNCTION FOR GROUND STATE

LHY had given a *physical picture* of the ground state Ψ_0. It turns out to be a collection of n pairs of particles floating in a sea of $\mathbf{k} = 0$ particles. Each pair consists of two particles with momenta $\mathbf{k}$ and $-\mathbf{k}$. The pair is not a bound pair, but a *correlated pair* with a correlation length equals to

$$r_0 = (8\pi a\rho)^{-1/2}. \tag{2}$$

$n = 0, 1, 2...$, with $n = 0$ being dominant, $n = 1$ the next dominant, etc. The average value of n is

$$\langle n\rangle = \frac{4N}{3\sqrt{\pi}}\sqrt{\rho a^3}. \tag{3}$$

Thus the probability of a particle being in $\mathbf{k} \neq 0$ state is $\frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3}$. Within one correlation length the number of particle is, on the average,

$$\sim \rho r_0^3 = \frac{1}{\sqrt{8\pi}^3}\frac{1}{\sqrt{\rho a^3}} \gg 1. \tag{4}$$

But most of these would be in the $\mathbf{k} = 0$ state, with only a few particle having $\mathbf{k} \neq 0$:

$$\sim \frac{1}{\sqrt{8\pi}^3}\frac{1}{\sqrt{\rho a^3}}\left[\frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3}\right] = \frac{1}{3\sqrt{8}\pi^2}.$$

In other words, within one correlation length, there are many particles, but only a few with $\mathbf{k} \neq 0$. The correlation therefore acts over a sea of particles almost all of which have $\mathbf{k} = 0$. That characteristic is, we believe, what was vaguely called momentum space ordering by London [5] in 1954 for a superfluid system.

It is interesting to compare the present theory for Bosons with the BCS theory for Fermions. In both cases there is *formation of correlated pairs*. But the mechanisms for the formation are quite different. The important common feature for the two cases is the presence of ODLRO [6].

PAIR DISTRIBUTION FUNCTION

The pair distribution function

$$D(r_{12}) \;=\; \rho^{-2}\langle\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)\rangle \tag{5}$$

is an important physical quantity *measurable* for many liquid systems. In this formula $\psi(\mathbf{r})$ is the annihilation operator in $\mathbf{r}$ space.

The pair distribution function $D(r_{12})$ is also related to the *diagonal elements* of the reduced density matrix [6]:

$$D(r_{12}) = \rho^{-2}\text{Trace}[\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)\rho_N\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)],$$

where $\rho_N = \Psi_0\Psi_0^\dagger$.

The meaning of $D(r)$ is: given a particle at a point, the average number of particles in $d^3\mathbf{r}$ at a distance r is $\rho D(r)d^3\mathbf{r}$. Thus $D(r) \to 1$ as $r \to \infty$.

For the dilute Bose system under consideration, $D(r)$ has been [7] computed in LHY:

$$D(r) = [1 + G(r)]^2 + [1 + F(r)]^2 - 1 - 2f[G(r) + F(r)] \tag{43'}$$

where

$$F(r) \;=\; \frac{1}{8\pi^3\rho}\int\frac{\alpha^2}{1-\alpha^2}e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k},$$
$$G(r) \;=\; -\frac{1}{8\pi^3\rho}\int\frac{\alpha}{1-\alpha^2}e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k}. \tag{44}$$

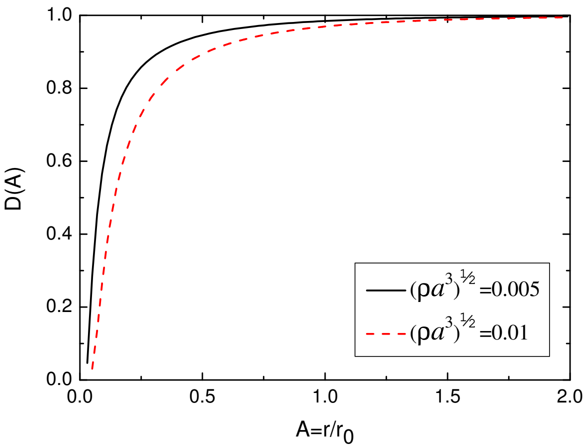

FIG. 1: (color online) Plot of $D(r/r_0)$.

The quantity α was defined in LHY by [38]. All equations with [ ] refer to equations in LHY. Converting the integrals $\int d^3\mathbf{k}$ into radial and angular parts yield

$$
\begin{aligned}
F(r) &= \frac{8}{A}\sqrt{\frac{2\rho a^3}{\pi}} I_1(A), \\
G(r) &= -\frac{8}{A}\sqrt{\frac{2\rho a^3}{\pi}} I_2(A), \qquad (6)
\end{aligned}
$$

$$
A = r/r_0, \quad r_0 = (8\pi a\rho)^{-\frac{1}{2}}, \qquad [45]
$$

where

$$
\begin{aligned}
I_1(A) &= \int_0^\infty \frac{\alpha^2}{1-\alpha^2}\xi d\xi \sin(A\xi), \\
I_2(A) &= \int_0^\infty \frac{\alpha}{1-\alpha^2}\xi d\xi \sin(A\xi), \qquad (7)
\end{aligned}
$$

and $\qquad \alpha = 1 + \xi^2 - \sqrt{(1+\xi^2)^2 - 1}.$

We plot [7] $D(r)$ for several values of $\sqrt{\rho a^3}$ in Fig. 1.

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[7] We noticed that equations [46] in LHY are in error. They should read, for $r \gg r_0$, $F(r) \to -G(r) \to \frac{1}{4\sqrt{2}}[\pi^2\rho r_0 r^2]^{-1}$. Also [43] in LHY is in error. It should read as [43′] in the present note.